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How AD can help solve differential-algebraic equations

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A characteristic feature of differential-algebraic equations is that one needs to find derivatives of some of their equations with respect to time, as part of the so-called index reduction or regularization, to prepare them for numerical solution. This is often done with the help of a computer algebra system. We show in two significant cases that it can be done efficiently by pure algorithmic differentiation. The first is the Dummy Derivatives method; here we give a mainly theoretical description, with tutorial examples. The second is the solution of a mechanical system directly from its Lagrangian formulation. Here, we outline the theory and show several non-trivial examples of using the 'Lagrangian facility' of the Nedialkov–Pryce initial-value solver DAETS, namely a spring-mass-multi-pendulum system; a prescribed-trajectory control problem; and long-time integration of a model of the outer planets of the solar system, taken from the DETEST testing package for ODE solvers.

Keywords: algorithmic differentiation; differential-algebraic equations; dummy derivatives; Lagrangians

1. Introduction

1.1 *DAE formulation and basic ideas*

In industrial engineering, the modelling of systems to simulate their time evolution is increasingly done by methods that lead to a differential-algebraic equation (DAE) system as the underlying mathematical form. Such DAEs often come from equation-based modelling (EBM), which describes system components by the basic physical laws they obey and supports 'multi-physics' models that combine several scientific disciplines, as for instance mechanical, electrical, chemical, and thermodynamic behaviour in a car engine.

Facilities created to support EBM include gPROMS, which is both a language and a graphical modelling environment (GME) built on it; the Modelica language and GMEs such as OpenModelica, Dymola and MapleSim that are built on it. Simulink, built on MATLAB, is a GME of similar scope but less in tune with the general DAE concept.

A DAE is just a set of n equations connecting a vector $\mathbf{x} = \mathbf{x}(t)$ of n state variables $x_1, \ldots, x_n$ and some derivatives of them with respect to time t. One can always reduce it to a first-order form $\mathbf{F}(t, \mathbf{x}, \dot{\mathbf{x}}) = 0$—as accepted by the DASSL solver and its relatives [1,7]—in the same way

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as one does for an ODE system. Here $\dot{\mathbf{x}}$ means $\mathrm{d}\mathbf{x}/\,\mathrm{d}t$. However we use a more flexible form allowing arbitrary higher derivatives:

$$f_i(t,\ \text{the } x_j \text{ and derivatives of them}) = 0, \quad i = 1, \ldots, n. \tag{1}$$

This often lets one formulate problems to our DAETS initial-value code [11,12] more concisely, e.g. Lagrange's equations for a mechanical system with n_q coordinates and n_c constraints need $n_q + n_c$ variables, compared to $2n_q + n_c$ in the first-order form.

1.2 *Aim*

In general, differentiating some of DAE's equations $f_i = 0$ with respect to t is an essential step in solving a DAE. This article is about two significant and rather different uses of this. The first is the widely used dummy derivatives (DDs) method of Mattsson and Söderlind [8] that prepares a higher index DAE for numerical solution by a classical index-1 DAE code, or by an explicit ODE code such as a Runge–Kutta method.

The second is the task of solving a, possibly constrained, mechanical system directly from a Lagrangian formulation. Conceptually it has several phases. The motion is defined by a Lagrangian function $L(t, \mathbf{q}, \dot{\mathbf{q}})$ where $\mathbf{q}$ is a vector of generalized coordinates q_i, plus possibly a vector of n_c constraints $\mathbf{C}(t, \mathbf{q}) = \mathbf{0}$. To set up (phase 1), the equations of motion from L and C one applies partial differentiation $\partial/\partial q$ and $\partial/\partial \dot{q}$, as well as straight $\mathrm{d}/\mathrm{d}t$, to L and C. When $n_c > 0$ the result is an index 3 DAE, which must (phase 2) be readied for numerical solution and (phase 3) solved.

Either use case at first sight seems to need symbolic differentiation, e.g. in a computer algebra system. We show pure AD suffices in either case. This insight may not be new but we believe the method is: for DDs it is new to combine index and order reduction in one simple framework; for Lagrangian calculations it is new to combine all phases seamlessly by AD, giving a simple user interface and efficient numerical solution.

2. Structural analysis

In an ODE $\dot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x})$, causality is obvious: in differential language, it explicitly specifies the state $\mathbf{x} + \mathrm{d}\mathbf{x}$ at the next instant $t + \mathrm{d}t$ to be $\mathbf{x} + \mathbf{f}(t, \mathbf{x})\,\mathrm{d}t$.

In a DAE, causality is not obvious. For instance, these size 2 DAEs are quite different, where $u(t)$ is a given driving function:

$$x_1 - u(t) = 0, \quad x_1 - \dot{x}_2 = 0, \tag{2}$$

$$\text{and} \quad x_2 - u(t) = 0, \quad x_1 - \dot{x}_2 = 0. \tag{3}$$

To solve (2), make $\dot{x}_2$ the subject of its second equation (x_1 causes x_2) and integrate the result; it is really an ODE, with one degree of freedom. To solve (3), make x_1 the subject of its second equation (x_2 causes x_1) and differentiate. DAE (3) has no degrees of freedom—it has the unique solution $x_1 = \dot{u}(t)$, $x_2 = u(t)$ and does not look like an ODE at all; such behaviour is common in control problems.

A solvable DAE has a chain of causality that must be found in order to prepare for numerical solution. Knowing which equations $f_i = 0$ to differentiate, and how often, is crucial to finding this causal chain. When correctly done, the original DAE augmented by the differentiated equations

can be solved to produce an ODE in some (possibly not all) of the original variables—the ODE part. Once this ODE is solved, the remaining variables forming the algebraic part can be found by algebraic manipulations combined with differentiations.

Let c_i be the number of differentiations of equation i needed by the 'most economical' way of doing this. For reasons to do with the Taylor series method used by DAETS we call them the *equation-offsets*.

For instance the equations of (2) do not need differentiating: $(c_1, c_2) = (0, 0)$. We solve to produce the ODE part $\dot{x}_2 = u(t)$ in just x_2. By contrast, (3) has $(c_1, c_2) = (1, 0)$ meaning the first equation must be differentiated, after which we solve to get $x_1 = \dot{u}(t)$, $x_2 = u(t)$. The ODE part is empty.

In the DAE (2), it happens we can solve for the algebraic variable x_1 to get $x_1 = u(t)$, independently of solving the ODE, but this need not be so: if we change it to

$$x_1 - x_2 - u(t) = 0, \quad x_1 - \dot{x}_2 = 0, \tag{4}$$

then the ODE part, namely $\dot{x}_2 - x_2 - u(t) = 0$, must be solved before we know x_1.

Unlike a well-behaved ODE $\dot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x})$, which has a solution path through each point of the region R of $(t, \mathbf{x})$ space where it is defined, the union of a typical DAE's solution paths is a proper subset of R, the *consistent manifold* $\mathcal{M}$ or set of *consistent points*. The dimension of its intersection with any time $t = t_0$ is DOF, the number of *degrees of freedom*, equivalently the size of its ODE part (here assumed independent of t_0).

The *index* of a DAE used in this paper is simply

$$\nu = \max_i c_i. \tag{5}$$

The classical *differentiation index* ν_d of Brenan *et al.* [1] assigns index 1 to DAE (2) and 2 to DAE (3). In summary for the examples above

DAE	ODE part	DOF	algebraic part	offsets	ν	ν_d
Equation (2)	x_2	1	x_1 (found independently of ODE part)	$(0, 0)$	0	1
Equation (3)	empty	0	x_1, x_2	$(1, 0)$	1	2
Equation (4)	x_2	1	x_1 (found using x_2 in ODE part)	$(0, 0)$	0	1

The *structural analysis* (SA) approach aims to derive a DAE's causal chain by studying its sparsity, namely what derivatives of variables occur in what equations. The method is: seek a number c_i of times to differentiate the ith equation that gives a structurally nonsingular (SNS) set of equations for the resulting highest, d_jth, derivatives of the x_j—then $\mathbf{c} = (c_1, \ldots, c_n)$, $\mathbf{d} = (d_1, \ldots, d_n)$ are the vectors of equation-offsets and corresponding variable-offsets. SNS means one can make a matching of variables to equations—equivalently a transversal, a set T of n positions (i, j) in an $n \times n$ matrix with just one in each row and in each column—such that derivative $x_j^{(d_j)}$ occurs in the differentiated equation $f_i^{(c_i)} = 0$ for each $(i, j) \in T$. There exist unique element-wise smallest non-negative $\mathbf{c}, \mathbf{d}$, the canonical offsets, which we assume chosen henceforth. They define the 'most economical' differentiations mentioned above.

An *SA-friendly* DAE by definition is one for which these equations are actually (not just structurally) nonsingular at some consistent point, that is, the $n \times n$ *system Jacobian*

$$\mathbf{J} = \left(\partial f_i^{(c_i)} / \partial x_j^{(d_j)}\right)_{i,j=1,\ldots,n}. \tag{6}$$

is nonsingular there. Assuming suitable smoothness of the f_i, a unique solution then exists locally through this point, and through any nearby consistent points.

Experience shows most DAEs in practice are SA-friendly. This fact underlies the wide use of the DDs method, which uses the results of SA and succeeds if and only if the DAE is SA-friendly. The SA can be done by the graph-based Pantelides method [14], or the Pryce Σ-method [15] based on the signature matrix $\Sigma = (\sigma_{ij})$, where

$$\sigma_{ij} = \begin{cases} \text{order of highest derivative of } x_j \text{ in } f_i & \text{if } x_j \text{ occurs in } f_i, \\ -\infty & \text{if not.} \end{cases} \tag{7}$$

The methods are equivalent except that the latter handles higher order DAEs without reduction to first order, while the former as described in [14] does not.

The DAE (with index $\nu_d = 3$) derived from a constrained Lagrangian of a mechanical system as in Section 4, is always SA-friendly when posed as an initial value problem. Posed otherwise, e.g. as a prescribed-trajectory control problem, it need not be. The occurrence of non-SA-friendly but solvable DAEs in applications is studied in [16,18]. For systematic ways of converting such a DAE to an equivalent SA-friendly one see [20].

SA leads to a notion of structural index ν_s, defined as the ν in (5), plus 1 if any offset d_j is zero. For an SA-friendly DAE ν_s is always $\geq \nu_d$, and usually equals it in practice, see [15].

3. Dummy derivatives

3.1 *The DDs construction*

Many numerical methods for higher index DAEs start with index reduction: augmenting the DAE by time-derivatives of some of its equations to produce a DAE of larger size and smaller index. Various index reduction methods have been used that convert the DAE to an ODE with more degrees of freedom than the DAE. Then the DAE's solution paths form a proper subset of those of the ODE. This tends to be bad numerically, as errors cause drift from the consistent manifold that can be exponential once it starts.

Dummy derivatives (DDs) by contrast are a systematic way to form an equivalent ODE with *exactly as many* DOF as the (SA-friendly) DAE. If one views the DAE as a flow on the consistent manifold $\mathcal{M}$, DDs describe the flow in a local coordinate system for $\mathcal{M}$. Thus numerical drift can only be within $\mathcal{M}$, where it is less harmful. However if the path leaves the patch of $\mathcal{M}$ where the coordinate system is nonsingular, one must choose new coordinates. This need for DD *switching*, or *pivoting*, complicates a numerical algorithm.

The following description of the DDs process is equivalent to that in [8]. The set of possible matrix sequences $(\mathbf{G}_k)$ whenever one selects a state vector, below, is the same in either method, but we find $\mathbf{G}_k$ from smallest up (each is a sub-matrix of the next), while [8] finds them in the opposite order.

Assume c_i and d_j are the canonical offsets. First form the derivatives of each $f_i = 0$ up to the c_ith, forming the augmented system of $N_f = n + \sum_i c_i$ equations:

$$f_i^{(l)} = 0, \quad l = 0, \ldots, c_i, \;\; i = 1, \ldots, n. \tag{8}$$

Its unknowns are the $N_x = n + \sum_j d_j$ derivatives of the state variables x_j up to the d_jth. View them for now as unrelated algebraic unknowns that we call items, and to emphasise this denote them x_{jl}:

$$x_{jl} \text{ renames } x_j^{(l)}, \quad l = 0, \ldots, d_j, \;\; j = 1, \ldots, n. \tag{9}$$

The system has fewer equations than variables by the amount $\sum_j d_j - \sum_i c_i$, which equals the number DOF of degrees of freedom. To balance this, the DDs method finds a number DOF of items x_{jl} to be state items, for (j, l) in a suitable set S of index pairs, chosen such that all the other items can locally be solved for as functions of these. The state vector $\mathbf{x}_S$ formed by the state items is the associated local coordinate system of the manifold $\mathcal{M}$.

One requires $l < d_j$ for each $(j, l) \in S$, so that $x_{j,l+1}$ is also an item. Then the differential relations between each state item and its next higher derivative:

$$\dot{x}_{jl} = x_{j,l+1} \tag{10}$$

can be interpreted as an ODE system for the state items.

State vector selection—initially or at a DD-switching point—may be done as follows. The $n \times n$ system Jacobian $\mathbf{J}$ in Equation (6) is nonsingular there. For $k = k_\mathrm{d}, k_\mathrm{d} + 1, \ldots, -1$ where k_d is minus the largest d_j, the 'standard solution scheme' of the Σ-method constructs sub-matrices $\mathbf{J}_k$ of $\mathbf{J}$ by selecting those rows i where $k + c_i \geq 0$ and columns j where $k + d_j \geq 0$. Then: $\mathbf{J}_k$ is of full row rank; it has size $m_k \times n_k$ where $m_k \leq n_k$; the sum of the differences $\sum_k (n_k - m_k)$ equals DOF. For each k, select m_k columns of $\mathbf{J}_k$ that form a nonsingular matrix $\mathbf{G}_k$. This can and must be done in such a way that the set of selected columns increases with k, so that each $\mathbf{G}_k$ is a sub-matrix of the next. For each of the $(n_k - m_k)$ unselected columns j consider the item $x_j^{(k+d_j)}$. The set of all these is a valid state vector $\mathbf{x}_S$ since, briefly, non-singularity of $\mathbf{G}_k$ ensures that at stage k, 'selected' items $x_j^{(k+d_j)}$ belonging to selected columns can, by the Implicit Function Theorem, be found locally as functions of the unselected items.

As said, (10) thus becomes a size- DOF ODE system,

$$\dot{\mathbf{x}}_S = \mathbf{F}(t, \mathbf{x}_S). \tag{11}$$

This is locally equivalent to the size-N_x DAE (8), (10) and hence to the original DAE. Though 'index-1' is the usual term used, the stronger property holds that

(8), (10) form an *implicit ODE*,

defined as an SA-friendly DAE whose offsets c_i are all zero.

3.2 *Example*

Example 3.1 (Pendulum) Let the original DAE be the simple pendulum in cartesian coordinates, shown with its signature matrix (7), with relevant transversals marked. Gravity g and

length ℓ are constants, and $x(t)$, $y(t)$ and $\lambda(t)$ are state variables.

$$\begin{aligned} 0 &= A = \ddot{x} + x\lambda, \\ 0 &= B = \ddot{y} + y\lambda - g, \\ 0 &= C = x^2 + y^2 - \ell^2, \end{aligned} \qquad \Sigma = \begin{array}{c} \\ A \\ B \\ C \\ d_j \end{array} \begin{array}{c} \begin{array}{cccc} x & y & \lambda & c_i \end{array} \\ \begin{bmatrix} 2^\bullet & & 0^\circ \\ & 2^\circ & 0^\bullet \\ 0^\circ & 0^\bullet & \end{bmatrix} \begin{array}{c} 0 \\ 0 \\ 2 \end{array} \\ \begin{array}{ccc} 2 & 2 & 0 \end{array} \end{array} \tag{12}$$

The offsets $c_i = 0, 0, 2$ imply C is to be differentiated twice, giving 5 equations in 7 unknowns. On the left of (13), these are shown in the notation of (12); on the right they have been translated to the general x_{jl} notation where x is called variable 1 so its derivatives $x, \dot{x}, \ddot{x}$ become x_{10}, x_{11}, x_{12}, and so on. The functions A,B,C are renamed as f's and a similar notation used for their derivatives.

Augmented system	After renaming
$0 = A = \ddot{x} + x\lambda$	$0 = f_{10} = x_{12} + x_{10}x_{30}$
$0 = B = \ddot{y} + y\lambda - g$	$0 = f_{20} = x_{22} + x_{20}x_{30} - g$
$0 = C = x^2 + y^2 - \ell^2$	$0 = f_{30} = x_{10}^2 + x_{20}^2 - \ell^2$
$0 = \dot{C} = 2(x\dot{x} + y\dot{y})$	$0 = f_{31} = 2(x_{10}x_{11} + x_{20}x_{21})$
$0 = \ddot{C} = 2(x\ddot{x} + \dot{x}^2 + y\ddot{y} + \dot{y}^2)$	$0 = f_{32} = 2(x_{10}x_{12} + x_{11}^2 + x_{20}x_{22} + x_{21}^2)$
unknowns $x, \dot{x}, \ddot{x}, y, \dot{y}, \ddot{y}, \lambda$	unknowns $x_{10}, x_{11}, x_{12}, x_{20}, x_{21}, x_{22}, x_{30}$

(13)

One can choose any of $(x, \dot{x})$, $(y, \dot{y})$, $(x, \dot{y})$, $(y, \dot{x})$ as state vector (one *must* choose one undifferentiated variable and one first derivative), but only the first two are 'convenient' for AD, as the next section shows.

Suppose for example $\mathbf{x}_S = (x, \dot{x}) \equiv (x_{10}, x_{11})$. It is easily seen that provided y, i.e. x_{20}, is nonzero one can find all the items as functions of these two, hence the pendulum DAE is equivalent to an ODE (11) in this $\mathbf{x}_S$ when $y \neq 0$.

The description of DDs given in Section 3.1 has the advantage of combining index reduction and order reduction into one process. For computer solution, it is probably easiest to work with the order 1 DAE formed by the $N_x = n + \sum_j d_j$ Equations (8), (10). However 'by hand', one can simplify by directly substituting the derivative relations into (8) where possible. E.g. the right-hand set of equations of (13) becomes

$$\begin{aligned} 0 &= A_0 = \dot{x}_{11} + x_{10}x_{30}, \\ 0 &= B_0 = x_{22} + x_{20}x_{30} - g, \\ 0 &= C_0 = x_{10}^2 + x_{20}^2 - \ell^2, \\ 0 &= C_1 = 2(x_{10}x_{11} + x_{20}x_{21}), \\ 0 &= C_2 = 2(x_{10}\dot{x}_{11} + x_{11}^2 + x_{20}x_{22} + x_{21}^2), \\ 0 &= \dot{x}_{10} - x_{11}. \end{aligned}$$

In the first equation, x_{12} has become $\dot{x}_{11}$. The last equation, $\dot{x}_0 = x_1$, can not be 'substituted away'—in general, any Equation (10) must stay if its x_{jl} and $x_{j,l+1}$ are both state items, as this is how order reduction occurs.

In Mattsson and Söderlind's [8] terminology, a 'dummy derivative' means a differentiated item that, in our terms, is a solved for item but is not a state variable or the derivative of one. In this example with this state vector, that makes y_1 and y_2 the DDs.

3.3 *Issues with switching, and numerical solution method*

At a DD-switch, the set (8) of differentiated equations does not change. Thus at the housekeeping level, a switch merely changes the set S of index pairs (j, l) that define the state vector. We verified that this switching method works, by a proof-of-concept MATLAB implementation, as well as one in C++ to verify the AD aspects. One example was the double pendulum (one pendulum-rod hung off another) in x,y coordinates, where each rod independently has four DD-switching points in a full rotation, one in each quadrant, giving $4 \times 4 = 16$ possible 'DD modes'.

It remains to be seen how efficient one can make DD-switching for production code and for larger problems. Finding the $\mathbf{G}_k$ at a switch is non-trivial. Ideally one wants each one to be maximally well-conditioned, which is expensive, so one seeks heuristic methods. This makes Scholz and Steinbrecher's simplified method [17] interesting. Less general than full DDs but cheaper, it uses a highest-value transversal of the signature matrix to find a state vector. One might try it first, and if it gives ill-conditioned $\mathbf{G}_k$, use full DDs.

It seems natural to solve the original DAE numerically, by giving formulation (8), (10) to a standard index-1 DAE solver. However many models, especially mechanical ones, have many equations but few degrees of freedom, $N_x \gg$ DOF. Then it makes sense to convert to the explicit ODE form (11). In many mechanical contexts (though not all) this ODE is non-stiff and thus amenable to, say, an explicit Runge–Kutta method. Working memory for sub-problems of size up to n is needed by the root-finding that forms (11), but is typically less than that needed by an implicit DAE code on a problem of size N_x.

3.4 *AD for DDs*

How can an AD tool help automate numerical solution by DDs, as described above?

It is helpful, but not essential, if the tool supports $\mathrm{d}/\mathrm{d}t$ as a first-class operator, of equal status with $+, \times, \sin()$, etc., so that it can understand a representation of a DAE in the general form (1). Tools such as ADOL-C and dcc/dco [5,9] do not have this feature, but can handle arbitrary expressions containing derivatives by renaming the latter as algebraic items and stating their differential relations separately. This is like the method in Section 3.1, where derivatives are renamed as algebraic in (9) and some differential relations between them stated in (10).

Our solver DAETS uses Ole Stauning's AD package FADBAD++ [19], written in C++. It did not originally include $\mathrm{d}/\mathrm{d}t$ but at our request in 2002, Stauning included the operator `Diff` such that `Diff(`$\cdot, q$`)` means $\mathrm{d}^q/\mathrm{d}t^q$. For instance, straightforward code for the pendulum, as in the DAETS user guide, is shown in Figure 1.

More important, for DDs and other index reduction methods, an AD tool must be able to differentiate the f_i selectively. For instance in the pendulum, A and B are to be left alone, and C differentiated twice.

```
1  template <typename T>
2  void fcn(T t, const T *z, T *f, void *param) {
3   // z[0], z[1], z[2] are x, y, λ.
4   const double G = 9.81, L = 10.0;
5   f[0] = Diff(z[0],2) + z[0]*z[2];
6   f[1] = Diff(z[1],2) + z[1]*z[2] - G;
7   f[2] = sqr(z[0]) + sqr(z[1]) - sqr(L);
8  }
```

Figure 1. Code for simple pendulum problem.

At first sight this seems to require a tool based on source code transformation, which could generate code symbolically for the last two equations in (13), for instance. But this is not so—the key is to treat different derivatives of a given variable, not in isolation but stored together as a truncated power series (storage in DAETS is already organized this way). For instance in the pendulum, the unknowns form three objects

$$\begin{array}{lll} \mathsf{x} & = (\mathsf{x}_0, \mathsf{x}_1, \mathsf{x}_2) & \text{order 2 power series,} \\ \mathsf{y} & = (\mathsf{y}_0, \mathsf{y}_1, \mathsf{y}_2) & \text{order 2 power series,} \\ \lambda & = (\lambda_0) & \text{order 0 power series.} \end{array}$$

Here and in the next two paragraphs, sanserif denotes that the series is represented by Taylor coefficients (usually more convenient for implementation), not derivatives, thus x_k relates to the x_k in (13) by $\mathsf{x}_k = x_k/k!$, and so on.

AD by overloading, provided by many AD tools, now gives the needed values. For instance evaluating $\mathsf{C} = \mathsf{x}^2 + \mathsf{y}^2 - \ell^2$ proceeds via these intermediate steps:

input		
x		$= (\mathsf{x}_0, \mathsf{x}_1, \mathsf{x}_2)$
y		$= (\mathsf{y}_0, \mathsf{y}_1, \mathsf{y}_2)$
compute		
v_1	$= \mathsf{x}^2$	$= (\mathsf{x}_0^2, \quad 2\mathsf{x}_0\mathsf{x}_1, \quad 2\mathsf{x}_0\mathsf{x}_2 + \mathsf{x}_1^2)$
v_2	$= \mathsf{y}^2$	$= (\mathsf{y}_0^2, \quad 2\mathsf{y}_0\mathsf{y}_1, \quad 2\mathsf{y}_0\mathsf{y}_2 + \mathsf{y}_1^2)$
v_3	$= \mathsf{v}_1 + \mathsf{v}_2$	$= (\mathsf{x}_0^2 + \mathsf{y}_0^2, \quad 2(\mathsf{x}_0\mathsf{x}_1 + \mathsf{y}_0\mathsf{y}_1), \quad 2(\mathsf{x}_0\mathsf{x}_2 + \mathsf{y}_0\mathsf{y}_2) + \mathsf{x}_1^2 + \mathsf{y}_1^2)$
C	$= \mathsf{v}_3 - \text{const}(\ell^2)$	$= (\mathsf{x}_0^2 + \mathsf{y}_0^2 - \ell^2, \quad 2(\mathsf{x}_0\mathsf{x}_1 + \mathsf{y}_0\mathsf{y}_1), \quad 2(\mathsf{x}_0\mathsf{x}_2 + \mathsf{y}_0\mathsf{y}_2) + \mathsf{x}_1^2 + \mathsf{y}_1^2)$

returning a degree 2 power series object C holding the needed coefficients $(\mathsf{C}_0, \mathsf{C}_1, \mathsf{C}_2)$, that is $(C, \dot{C}, \frac{1}{2}\ddot{C})$ in terms of derivatives.

Evaluating $A = \ddot{x} + x\lambda$ and $B = \ddot{y} + y\lambda - g$ is similar. Differentiating twice converts, e.g. the degree 2 series $\mathsf{x} = (\mathsf{x}_0, \mathsf{x}_1, \mathsf{x}_2)$ to the degree 0 series $(2\mathsf{x}_2)$. Thus A and B are returned as the degree 0 series $\mathsf{A} = (\mathsf{A}_0) = (2\mathsf{x}_2 + \mathsf{x}_0\lambda_0)$ and $\mathsf{B} = (\mathsf{B}_0) = (2\mathsf{y}_2 + \mathsf{y}_0\lambda_0 - g)$.

The above method gives an explicit evaluation of the N_f functions (8) at the N_x arguments (9). In the DDs context of reducing the DAE to an explicit ODE, one inputs state item values, say $\mathbf{x}_S = (x_0, x_1)$. The 5 items $\mathbf{x}_F = (x_2, y_0, y_1, y_2, \lambda_0)$ are trial values that produce 5 residual values $\mathbf{r} = (A_0, B_0, C_0, C_1, C_2)$. By root-finding using suitable Jacobians, see below, we find $\mathbf{x}_F$ that makes $\mathbf{r} = \mathbf{0}$, thus solving for $\mathbf{x}_F$ as a function of $\mathbf{x}_S$. Extract x_2 from $\mathbf{x}_F$ to form (x_1, x_2), which is $\dot{\mathbf{x}}_S$. This implements $\mathbf{F}$ in (11).

To make this work, the state items must comprise a contiguous set of derivatives of each variable, with no gaps. (Hence, cf. the paragraph following (13), $(x, \dot{y})$ and $(y, \dot{x})$ are not useful state vectors for the pendulum.) That is, S must have the form $\{\,(j,l) \mid 0 \le l < \delta_j, j = 1, \ldots, n\,\}$, where $\boldsymbol{\delta} = (\delta_1, \ldots, \delta_n)$ is an integer DD-spec vector with $0 \le \delta_j \le d_j$ and $\sum_j \delta_j = \text{DOF}$, which uniquely specifies the DD scheme currently in use. DD switching can be based on changing this $\boldsymbol{\delta}$, and following through the consequences for various associated index sets and Jacobian-related matrices.

3.4.1 *Complexity and efficiency aspects*

We assume—see Section 3.3—numerical solution is by reducing (8), (10) to explicit ODE form (11) and using an explicit ODE solver. To use an implicit, e.g. stiff, solver and compute exact Jacobians $\partial\mathbf{F}/\partial\mathbf{x}_S$ for this by AD is more challenging.

Function values (8). Denote the vector of functions f_i in (1) by $\mathfrak{f}$, with inputs $(t, \mathbf{x})$ where $\mathbf{x}$ denotes relevant 'x_j and derivatives'. View $\mathfrak{f}$ as a computational graph or code list, overloaded to compute different things depending on the type of inputs given to it.

Let $\mathbf{x^{(d)}}$ denote the vector whose jth component is a degree d_j truncated Taylor Series (TS) of x_j, equivalently the list of x_j's derivatives up to the d_jth. E.g. for the pendulum we use $\mathbf{x^{(d)}} = (x, y, \lambda)^{((2,2,0))} = ((x, \dot{x}, \ddot{x}), (y, \dot{y}, \ddot{y}), (\lambda))$, or the corresponding list of Taylor coefficients. Let $\mathbf{f^{(c)}}$ have the similar meaning. Then evaluating (8) can be written as follows:

$$\mathbf{f^{(c)}} = \mathfrak{f}(t, \mathbf{x^{(d)}}). \tag{14}$$

with the rigorous interpretation that a numerical TS vector $\mathbf{x^{(d)}}$ is given as input to the code list, with each elementary operation overloaded to be a TS operation.

As the pendulum example illustrates, SA acts here as a scheduling algorithm: if one starts with $\mathbf{x^{(d)}}$, each operation receives inputs of just the right degree, so $\mathbf{f^{(c)}}$ is returned as final output. (A differentiation reduces TS degree, while for algebraic operations the output degree is the least of the input degrees.)

Since average degrees are typically low, say at most 3, the work $W(\mathbf{f^{(c)}})$ of an evaluation of (14) is a modest multiple of the work $W(\mathfrak{f})$ of a basic evaluation of the DAE (1), depending on how the AD is implemented but independent of n.

Jacobians. The offsets give (8) a block-triangular structure. Evaluating $\mathbf{F}$ in (11) uses this, solving subsystems of size m_k for $k = k_c, \ldots, 0$, where $k_c = -\max_i c_i$ and $m_{k_c} \leq \cdots \leq m_0 = n$. Block k's Jacobian $\mathbf{G}_k$ is a square sub-matrix of the $m_k \times n_k$ system Jacobian $\mathbf{J}_k$ for SA stage k, which is a sub-matrix of the overall Jacobian $\mathbf{J} = \mathbf{J}_0$.

Nedialkov's group has put in DAETS a forward-AD method to compute $\mathbf{J}$, taken from [10]. It also overloads the code list, propagating compressed gradients instead of Taylor series; one can write it as $\nabla\mathbf{f} = \mathfrak{f}(t, \nabla\mathbf{x})$ with an interpretation analogous to (14). By a topological sort one can arrange that the code list for $\mathbf{J}_k$ is an initial segment of that for $\mathbf{J}_{k+1}$, for each k. If dense linear algebra is used, the work $W(\mathbf{J})$ to evaluate $\mathbf{J}$ is of order $nW(\mathfrak{f})$. However we use sparse linear algebra which, with the compressed gradients, usually gives big speedups on larger problems.

In general each block of (8) is a nonlinear system, but the quasi-linearity analysis phase of SA (overloading $\mathfrak{f}$ yet again) finds which blocks are linear, with further efficiency gains.

Experience with the corresponding task in DAETS suggests that

- With standard methods used in stepping codes for finding a good initial guess for a nonlinear solve, typically 1–3 evaluations of $\mathbf{f^{(c)}}$ are needed for each $\mathbf{F}$ evaluation.
- With standard ways to re-use 'old' Jacobians one can average < 1 evaluation of $\mathbf{J}$ per time step.
- The linear algebra cost is negligible compared with the AD cost.

Experiments by Nedialkov, using the C++ AD infrastructure of DAETS, confirm this is a viable way to implement DDs; as yet we do not have performance results to report.

4. The Lagrangian

4.1 *Mechanics theory*

For mechanical systems, such as in robotics, equations of motion can often be conveniently derived from the system's Lagrangian function L. It is assumed there are conservative (energy preserving) forces such that one can define a potential energy V depending only on system position. Then $L = T - V$, where T is the system's total kinetic energy. Let the configuration at any

time be described by generalized coordinates $\mathbf{q} = (q_1, \ldots, q_{n_q})$ such that T is a function of $\dot{\mathbf{q}}$ and possibly $\mathbf{q}$, and V is a function of $\mathbf{q}$ only. There may (depending on the coordinate system used) be n_c scalar constraints that are holonomic, i.e. functions of positions and possibly time but not of velocities, namely $C_j(t, \mathbf{q}) = 0$.

Then the variational principle of stationary action gives the (n_q+n_c) Euler–Lagrange equations (ELEs) that describe the motion:

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} + \sum_{j=1}^{n_c} \lambda_j \frac{\partial C_j}{\partial q_i} = 0, \quad i = 1, \ldots, n_q, \tag{15}$$

$$C_j(t, \mathbf{q}) = 0, \quad j = 1, \ldots, n_c, \tag{16}$$

where the λ_j are Lagrange multipliers for the constraints. For a system subject to external forces, the zero right-hand sides of (15) are replaced by $u_i(t, \mathbf{q}, \dot{\mathbf{q}})$, $i = 1, \ldots, n_q$, which are generalized external force components.

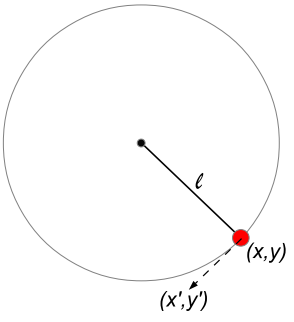
If $n_c > 0$, i.e. constraints are present, (15), (16) is termed a Lagrangian system of the first kind. It is a DAE system, of index 3 in the classical sense or index 2 as defined in (5), since two t-differentiations of each C_j are needed. If the coordinates are chosen so that $n_c = 0$, it is of the second kind and is an ODE system.

E.g. for free motion of the simple pendulum, taking $\mathbf{q} = (x, y)$, the cartesian coordinates of the pendulum bob (of mass m) with y downward, gives

$$\begin{aligned} T &= \tfrac{1}{2} m(\dot{x}^2 + \dot{y}^2), \qquad V = -mgy, \\ L &= T - V = \tfrac{1}{2} m(\dot{x}^2 + \dot{y}^2) + mgy \end{aligned} \tag{17}$$

with one constraint that we write

$$0 = C = \tfrac{1}{2}(x^2 + y^2 - \ell^2) \tag{18}$$



(19)

Then (15), (16), on dividing through by m, lead to the pendulum DAE

$$\left.\begin{aligned} 0 = A &= \ddot{x} + x\lambda \qquad \text{from } 0 = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} + \lambda\frac{\partial C}{\partial x}, \\ 0 = B &= \ddot{y} + y\lambda - g \qquad \text{from } 0 = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{y}} - \frac{\partial L}{\partial y} + \lambda\frac{\partial C}{\partial y}, \\ 0 = 2C &= x^2 + y^2 - \ell^2. \end{aligned}\right\} \tag{20}$$

On the other hand, taking $\mathbf{q}$ to be (θ), the angle of the pendulum from the downward vertical, gives $L = \frac{1}{2} m(l\dot{\theta})^2 + mgl\cos\theta$, with no constraints. Then (15), (16) lead to the ODE $\ddot{\theta} = -(g/l)\sin\theta$, which is equivalent to (20).

```
template <typename T>
void fcn( T t, const T *z, T *f, void *param ) {
  vector< B<T> > q(SIZEOFQ), qp(SIZEOFQ), C(SIZEOFC);
  init_q_qp(z, q, qp);
  double *p = (double *)param;
  double  m = p[0], g = p[1], l = p[2];
  B<T> x = q[0], y = q[1], xp = qp[0], yp = qp[1];
  B<T> L = 0.5 * m * (sqr(xp) + sqr(yp)) + m * g * y;
  C[0] = sqr(x) + sqr(y) - sqr(l);
  setupEquations(L, z, q, qp, C, f);
}
```

Figure 2. Code to describe pendulum in Lagrangian form.

4.1.1 *The Lagrangian facility in* DAETS

As said in Section 1.2, solution *apparently* comprises several phases: (1) Apply $\partial/\partial q$, $\partial/\partial \dot{q}$ and $\mathrm{d}/\mathrm{d}t$ on L and C to get the ELEs. (2) If these form a DAE, reduce index (e.g. by DDs) to prepare it for solution. (3) Solve it numerically. By using a high index solver for SA-friendly DAEs, we already merge phases 2 and 3. The new feature of the 'Lagrangian facility' is to merge phase 1 with these. We use DAETS with its built-in AD by FADBAD++; another DAE code with another AD system could do essentially the same.

The user describes a DAE system to DAETS by a function `fcn()` in which the mathematical variables become objects of a template type `T`, as Figure 1 in Section 3.4 shows. DAETS instantiates `T` during execution with various concrete types.

The user of the Lagrangian facility writes code for L instead of for the DAE equations. The generalized coordinates q_i become variables of a reverse differentiation type `B` built on top of `T`, that is `B`. In the pendulum example, these are the coordinates x,y which become `x`, `y` of type `B`, see Figure 2. The partial derivatives in the right of (18), as well as the $\mathrm{d}/\mathrm{d}t$, are computed by AD to obtain the equations on the left where the variables have been converted back to type `T`. The transformation, done in one direction by `init_q_qp()` and in the other by `setupEquations()`, is invisible to the user.

4.1.2 *Complexity and efficiency aspects*

For current symbolic approaches, see, e.g. [22], or webinar [21] for an introduction to Lagrangian modelling with MATLAB and SIMULINK. Using AD as we do to transform the Lagrangian has several advantages over these methods, besides user convenience:

- The complexity of computing a Taylor series of degree p from a code list (or computational graph, CG) of length l, using AD, is $O(p^2 l)$, but a straight symbolic approach often gives expressions that grow exponentially in p. Further, see, e.g. [4], the recursive expression for an ODE's or DAE's Taylor coefficients of degree r is jointly linear in the coefficients of degrees $> r/2$. Hence a TS of degree p can be computed in around $\log_2(p)$ sweeps though the CG, rather than the p sweeps of the most natural algorithm.
- This applies to the use of FADBAD++ as the AD package. The `fcn()` code is actually called only once for each instantiating type `T`. When `T` is Taylor mode, FADBAD++ converts this at run time to a CG representing the floating-point Taylor series evaluation, to the chosen degree (like the 'tape' used by the ADOL-C system).
  It optimizes this using methods of common-subexpression elimination (CSE) developed by Nedialkov's group, often significantly shortening the CG (see Table 2). The optimized CG is used by DAETS at each evaluation of functions (1) during numerical integration.

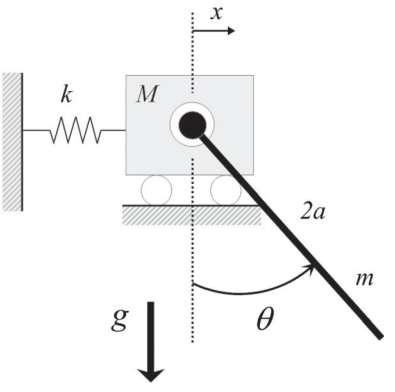


Figure 3. Spring-Mass-Pendulum with one rod.

This, with our efficient algorithm for System Jacobians and sparse linear algebra, mentioned in Section 3.4, often gives speedups of > 10 compared to `FADBAD++` without CSE.

4.2 *Examples*

We have applied the DAETS Lagrangian facility to various systems, including the following examples. Performance tests are on a 2017 MacBook Pro laptop with a 4-core 2.2 GHz Intel processor running Mac OS X 10.11.6. The `C++` compiler is `clang++` version 8.0.0. All numerics are in `C++ double`.

Visualisations of some results, produced in MATLAB from the DAETS output, can be viewed at the YouTube channel *Multi-body Lagrangian Simulations* [13] (Figure 3).

Because of the perceived difficulty of solving DAEs, generalized coordinates are often chosen to eliminate the constraints and give a Lagrangian of the second kind. For instance, a rigid body's 3D position can be described by 3 coordinates of the position of its centre of mass and 3 of its angular position relative to this. However the mathematical formulation is often simpler in cartesian coordinates. One plus of using a code for high-index DAEs such as DAETS is that it handles resulting 'first kind' systems easily. Further, since DAETS does not set up a local coordinate system for numerical solution as the DDs method does, it does not suffer the performance penalty of DD-switching.

Example 4.1 (Spring-Mass-Pendulum) This 2D model is taken from an article on the Acumen mechanics modelling system by Zhu, Taha *et al.* [22].

We have extended their model to a chain of any number n of rods. Namely, a horizontally sliding point-mass M is connected by a spring of stiffness k to a fixed point at the same level. From M hangs a chain of n uniform rods, with frictionless joints between the end of one and the start of the next. Purely to simplify the code, they all have the same mass m and length $l = 2a$. We assume the setup is constructed so that all components can slide or rotate freely without colliding.

For $n \geq 2$ (possibly even for $n = 1$), the motion can be chaotic. The figure (taken from [22]) shows the case $n = 1$. As the figure indicates, Zhu *et al.* [22] take $\mathbf{q} = (x, \theta)$ as coordinates, leading to a Lagrangian of the second kind, $L = T - V$ where:

$$T = \tfrac{1}{2}(M + m)\dot{x}^2 + ma\dot{x}\dot{\theta}\cos\theta + \tfrac{2}{3}ma^2\dot{\theta}^2, \quad V = \tfrac{1}{2}kx^2 + mga(1 - \cos\theta). \tag{21}$$

Here the rotational kinetic energy term $\frac{2}{3}ma^2\dot{\theta}^2$ uses the moment of inertia $I = \frac{4}{3}ma^2$ of a uniform rod about its centre of mass.

For the general n-rod model we use, instead, cartesian coordinates $\mathbf{q} = (x_0, x_1, \ldots, x_n;\ y_1, \ldots, y_n)$. Here $\mathbf{r}_0 = (x_0, y_0)$, with y_0 constant equal to 0, is the position of M and the start of rod 1, and $\mathbf{r}_i = (x_i, y_i)$ for $i = 1, \ldots, n$ is the position of the joint between the end of rod i and (for $i < n$) the start of rod $i+1$. We avoid moments of inertia by using the following, where $\cdot$ denotes the dot product of vectors.

LEMMA 4.1 *If the ends of a uniform rod of mass m have position vectors* r_0 *and* r_1, *depending on t, then its kinetic energy at any instant is*

$$\mathrm{KE} = \tfrac{1}{6}\, m(\dot{\boldsymbol{r}}_0 \cdot \dot{\boldsymbol{r}}_0 + \dot{\boldsymbol{r}}_0 \cdot \dot{\boldsymbol{r}}_1 + \dot{\boldsymbol{r}}_1 \cdot \dot{\boldsymbol{r}}_1).$$

Proof We can parameterize position along the rod as $\mathbf{r} = (1-s)\mathbf{r}_0 + s\mathbf{r}_1$, for $0 \le s \le 1$. Since the rod has total mass m, an element from s to $s + \mathrm{d}s$ has mass $m\,\mathrm{d}s$. The velocity of this element is $\dot{\mathbf{r}} = (1-s)\dot{\mathbf{r}}_0 + s\dot{\mathbf{r}}_1$ so its kinetic energy is

$$\tfrac{1}{2}\, m(\dot{\mathbf{r}} \cdot \dot{\mathbf{r}})\,\mathrm{d}s = \tfrac{1}{2}\, m\left((1-s)^2\ \dot{\mathbf{r}}_0 \cdot \dot{\mathbf{r}}_0 + 2(1-s)s\ \dot{\mathbf{r}}_0 \cdot \dot{\mathbf{r}}_1 + s^2\ \dot{\mathbf{r}}_1 \cdot \dot{\mathbf{r}}_1\right)\,\mathrm{d}s.$$

Integrating this from 0 to 1 gives the result. ■

The potential energy of the rods comes from considering the mass of rod i to be at its centre of mass at height $\frac{1}{2}(y_{i-1} + y_i)$; there is a contribution of $\frac{1}{2}kx_0^2$ from the spring and none from mass M. This leads to the Lagrangian $L = T - V$, and constraints C_i, where

$$\begin{aligned}
T &= \frac{1}{2}M\dot{x}_0^2 + \frac{1}{6}m\sum_{i=1}^{n}(\dot{\mathbf{r}}_{i-1}\cdot\dot{\mathbf{r}}_{i-1} + \dot{\mathbf{r}}_{i-1}\cdot\dot{\mathbf{r}}_i + \dot{\mathbf{r}}_i\cdot\dot{\mathbf{r}}_i)\\
&= \frac{1}{2}M\dot{x}_0^2 + \frac{1}{6}\,m\sum_{i=1}^{n}\left((\dot{x}_{i-1}^2 + \dot{y}_{i-1}^2) + (\dot{x}_{i-1}\dot{x}_i + \dot{y}_{i-1}\dot{y}_i) + (\dot{x}_i^2 + \dot{y}i^2)\right)\\
V &= \frac{1}{2}kx_0^2 + mg\sum_{i=1}^{n}\frac{1}{2}(y_{i-1}+y_i) = \frac{1}{2}kx_0^2 + mg\left(\frac{1}{2}y_n + \sum_{i=1}^{n-1}y_i\right),\\
0 = C_i &= (x_i - x_{i-1})^2 + (y_i - y_{i-1})^2 - \ell^2, \quad (i = 1, \ldots, n).
\end{aligned}$$

The code in Figure 4, which replaces lines 7–9 in the `fcn` of Figure 2, implements the above formulas. Here `n`, the number n of rods, is read in as one of the physical parameters. `SIZEOFC` also equals n. The arrays `q` and `qp` holding $\mathbf{q}$ and $\dot{\mathbf{q}}$ have length $2n+1$.

Listing line 1 uses `C` syntax[1] to split `q` into a scalar holding x_0, and two size-n arrays holding $x_1, \ldots, x_n$, and $y_1, \ldots, y_n$; similarly `qp`. The variable `KEsum` accumulates $\dot{x}_0^2 + \dot{x}_n^2 + \dot{y}_n^2 + \dot{x}_0\dot{x}_1 + \sum_{i=1}^{n-1}[2(\dot{x}_i^2 + \dot{y}_i^2) + \dot{x}_i\dot{x}_{i+1} + \dot{y}_i\dot{y}_{i+1}]$, which is equivalent to the sum in T, and similarly `PEsum`.

In the computation of `L`, the temporary dependent variables `KEsum`, `PEsum`, `KE`, and `PE`, are local in the block between lines 3 and 4; `FADBAD++` requires that in the reverse mode either all intermediate dependent variables are differentiated or go out of scope, which is the case here.

In our tests, the physical parameters of the original model in [22] were used, namely assuming SI units, $g = 9.8\,\mathrm{m\,s^{-2}}$, $l = 2a = 2\,\mathrm{m}$, $M = 5\,\mathrm{Kg}$, $m = 2\,\mathrm{Kg}$, $k = 10\,\mathrm{Kg\,s^{-2}}$.

The chosen initial conditions (ICs) are that the system is at rest with mass M at x_0=4, and the rods stretched horizontally to the left. (Thus the spring is pushing against the row of rods; animations show it 'folds up' rods 1 and 2 as they start to fall.)

To confirm that we are modelling the same system as in [22], the equations of motion derived from the Lagrangian (21) given in [22] were coded in MATLAB and integrated by `ode45`. The results were compared with those of the DAETS version for the case $n = 1$. The latter was coded

```
1   B<T> x0 = q[0], *x = q+1, *y = x+n, x0p = qp[0], *xp = qp+1, *yp = xp+n;
2    B<T> L;
3    {
4      B<T> KEsum = sqr(x0p) + sqr(xp[n-1]) + sqr(yp[n-1]) + x0p*xp[0];
5      for (int i=0; i < n-1; i++)
6        KEsum += 2*( sqr(xp[i]) + sqr(yp[i]) ) + xp[i]*xp[i+1] + yp[i]*yp[i+1];
7      B<T> KE = 0.5*M*sqr(x0p) + m/6*KEsum;
8
9      B<T> PEsum = 0.5*y[n-1];
10     for (int i=0; i<n-1; i++) PEsum += y[i];
11     B<T> PE = 0.5*k*sqr(x0) - m*g*PEsum;   // - as y goes downward
12
13     L = KE - PE;
14   }
15   C[0] = sqr(x[0]-x0) + sqr(y[0]) - sqr(l);
16   for (int i=1; i<SIZEOFC; i++)
17     C[i] = sqr(x[i]-x[i-1]) + sqr(y[i]-y[i-1]) - sqr(l);
```

Figure 4. Code for spring-mass-multi-pendulum system.

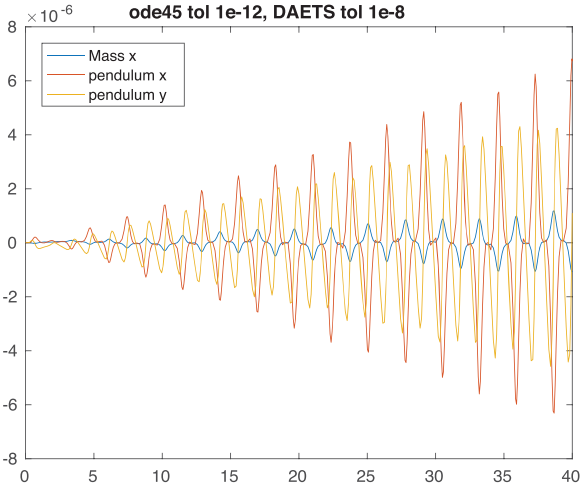


Figure 5. Spring-mass-pendulum with $n = 1$. It shows, for the x coordinate of the sliding mass and the x and y coordinates of the pendulum, the difference between the solution by our model and that by (19), over $0 \le t \le 40$.

Table 1. Time (seconds) to integrate to $t = 100$ for various numbers n of rods, and tolerances `tol`.

`tol`	$n=1$	2	4	6	8	10	12	14	16	18	20
1e−04	3.6e−02	1.2e−01	3.5e−01	7.3e−01	1.3	2.1	3.1	4.2	5.6	7.2	8.8
1e−06	4.5e−02	1.5e−01	3.8e−01	9.3e−01	1.8	2.8	4.3	5.5	7.9	9.9	12.0
1e−08	5.8e−02	2.3e−01	6.3e−01	1.3	2.4	3.7	5.6	7.7	10.0	13.3	16.5
1e−10	8.0e−02	2.7e−01	7.5e−01	1.7	3.1	4.8	7.7	10.9	13.8	17.4	22.3
1e−12	1.1e−01	4.3e−01	1.1	2.4	4.5	6.9	10.1	14.0	18.2	23.6	30.2

to output q and $\dot{q}$ at each of its time points t_i. These data were mapped to the t_i chosen by the MATLAB version by Hermite cubic interpolation between adjacent t_i of DAETS. Figure 5 shows that over $t = [0, 40]$, the differences (`ode45` solution at tolerance 10^{-12}) − (DAETS solution at tolerance 10^{-8}) are of order 10^{-6}. This gives confidence that the programs are solving the same physical model.

Table 2. Number of nodes in the computational graph of the spring-mass-pendulum example, without and with CSE.

n	1	2	4	6	8	10	12	14	16	18	20
without CSE	154	348	964	1884	3108	4636	6468	8604	11044	13788	16836
with CSE	120	211	415	649	915	1213	1543	1905	2299	2725	3183
% reduction	24.1	42.9	62.1	71.5	76.9	80.5	83.0	84.9	86.3	87.5	88.4

For timing tests, the system was integrated by DAETS over $0 \le t \le 100$ for various numbers n of rods and (mixed relative-absolute) tolerances `tol`. Case $n = 1$ is the model in [22]. The Taylor series degree was set to 15, which works well for these problems at this range of accuracies. Table 1 shows the times taken.

DAETS has a 'maximum step size' feature but this was not used so it chooses the step sizes h freely. For the 'hardest' problem $n = 20$ at tolerance 10^{-12}, they ranged from $h = 0.00061$ to $h = 0.09$. For the 'easiest', $n = 1$ at tolerance 10^{-4}, they ranged from $h = 0.09$ to $h = 0.83$.

In Table 2, we report the number of nodes in the CGs for the above number of rods: without CSE, with CSE, and the percentage of reduction in the number of nodes. Here it varies from 24.1% for $n = 1$ to 88.4% for $n = 20$.

Example 4.2 (Controlled simple pendulum) We show one can solve a prescribed-trajectory control problem for a Lagrangian-described system. Namely, for the simple pendulum we introduce a horizontal external force on the bob, modelled as a system input $u = u(t)$ such that the equation $\ddot{x} + \lambda x = 0$ becomes

$$\ddot{x} + \lambda x - u = 0. \tag{22}$$

The aim is to find $u(t)$ (plus suitable consistent ICs) so that the x position performs simple harmonic motion $x(t) = a\sin(\omega t)$ exactly, where the constants a and ω are a given amplitude and frequency, respectively.

Comparing the pendulum as initial-value problem in Figure 2 and as control problem in Figure 6 shows the implementation changes little. One passes a and ω as extra parameters that become `a` and `w`. After the `setupEquations` line, the first equation `f[0]` is modified in line 12, and a new fourth equation `f[3]` is at line 13 (in which the `x` at line 7 in Figure 2 cannot be used as it has the wrong type, `B` instead of `T`).

But the revision has changed the DAE's mathematical nature greatly. Now with 4 variables and equations, it is shown below with its signature matrix Σ (a blank means $-\infty$, and the unique transversal is marked by $^\circ$).

$$\begin{aligned} 0 = A &= x'' + x\lambda - u \\ 0 = B &= y'' + y\lambda - g \\ 0 = C &= x^2 + y^2 - \ell^2 \\ 0 = D &= x - a\sin(\omega t) \end{aligned} \qquad \Sigma = \begin{array}{c} \\ A \\ B \\ C \\ D \\ d_j \end{array} \begin{array}{c} \begin{array}{cccc} x & y & \lambda & u \end{array} & c_i \\ \left[\begin{array}{cccc} 2 & & 0 & 0^\circ \\ & 2 & 0^\circ & \\ 0 & 0^\circ & & \\ 0^\circ & & & \end{array}\right] & \begin{array}{c} 0 \\ 0 \\ 2 \\ 2 \end{array} \\ \begin{array}{cccc} 2 & 2 & 0 & 0 \end{array} & \end{array} \tag{23}$$

While (20) has 2 degrees of freedom, (23) has none—specifying the desired $x(t)$ determines the system input $u(t)$, as well as y and λ, uniquely.

With the physical parameters $g = 9.8$ and $\ell = 10$, the problem was solved by DAETS with ω equal to the pendulum's natural frequency $\sqrt{g/l}$ of small oscillations, and for various a; and again with ω changed by 20%, for the same a values. Some examples of resulting u's are plotted over several cycles in Figure 7. As expected, u is very small when ω is the natural frequency and

```
1  template <typename T>
2  void fcn( T t, const T *z, T *f, void *param ) {
3      vector< B<T> > q(SIZEOFQ), qp(SIZEOFQ), C(SIZEOFC);
4    init_q_qp(z, q, qp);
5    double *p = (double *)param;
6    double  m = p[0], g = p[1], l = p[2],
7      a = p[3], w = p[4];
8    B<T> x = q[0], y = q[1], xp = qp[0], yp = qp[1];
9    B<T> L = 0.5 * m * (sqr(xp) + sqr(yp)) + m * g * y;
10   C[0] = sqr(x) + sqr(y) - sqr(l);
11   setupEquations(L, z, q, qp, C, f);
12   f[0]-= z[3];
13   f[3] = z[0] - a*sin(w*t);
14 }
```

Figure 6. The `fcn` for the controlled pendulum problem: new lines 12 and 13 are inserted.

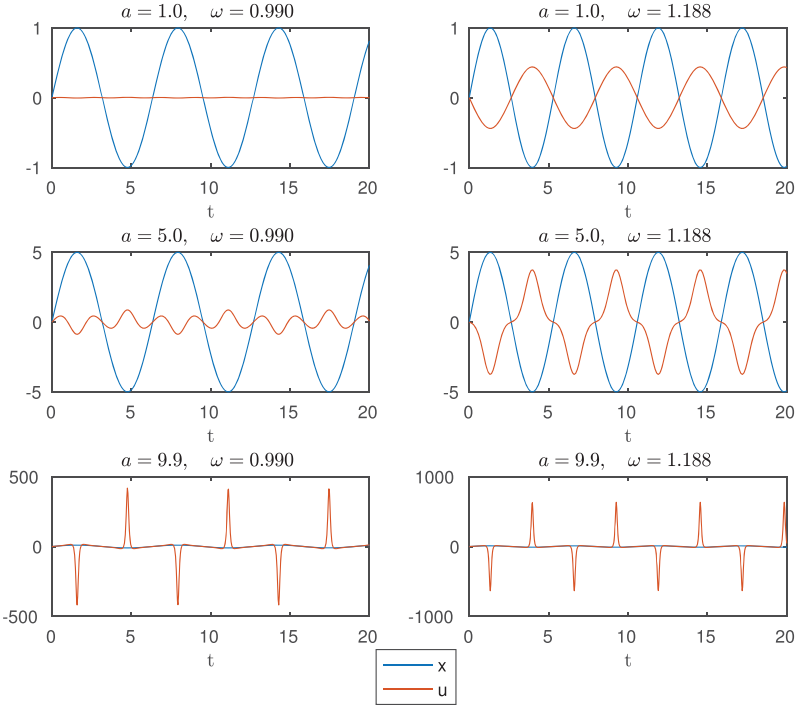


Figure 7. Solution by DAETS of system input $u(t)$ for controlled pendulum with $g = 9.8$, $l = 10$. Required response $x = a\sin(\omega t)$. For ω equal to natural angular frequency (left column) and 20% larger (right column), and three a values.

a is small. It becomes large as a approaches ℓ, or as the frequency moves away from the natural one. DAETS took less than 0.1 seconds for each of the runs.

Example 4.3 (DETEST Non-stiff Problem C5) This problem from the non-stiff part of the DETEST testing package for ODE solvers [2], and originally[2] from Zonneveld [23], is titled 'Five Body Problem: Motion of five outer planets about the Sun'. It is a order 2 ODE of size 15 (so size 30 when reduced to order 1), the variables being the positions of Jupiter, Saturn, Uranus, Neptune and Pluto relative to the Sun, in x,y,z coordinates such that the ecliptic plane, in which the orbits approximately lie, is not close to any of the three axes.

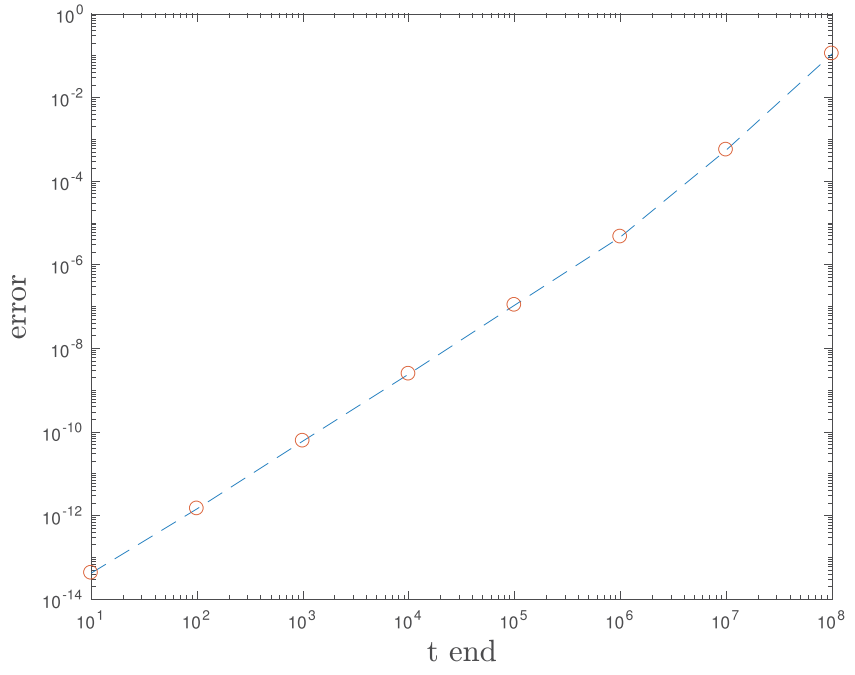


Figure 8. Log–log plot of divergence vs time. The planet model was integrated at two tolerances `1e-13` and `1e-15`. The norm of the difference between these solutions is plotted at 10^n TU, $n = 1, \ldots, 8$, showing no sign of chaotic behaviour for this set of ICs.

To set up the Lagrangian formulation, $\mathbf{q}$ comprising the 5 relative positions $(\boldsymbol{\varrho}_1(t), \ldots, \boldsymbol{\varrho}_5(t))$ (each $\boldsymbol{\varrho}$ being a 3-vector) is converted to 6 positions $(\mathbf{r}_0(t), \ldots, \mathbf{r}_5(t))$ of Sun and planets relative to their common centre of mass, which may be considered to be at rest in a Newtonian absolute frame. Namely let m_0 be the mass of the Sun and $m_1, \ldots, m_5$ the masses of the planets and subtract

$$\mathbf{r}_c = \frac{m_0\mathbf{0} + (m_1\boldsymbol{\varrho}_1 + \cdots + m_5\boldsymbol{\varrho}_5)}{m_0 + (m_1 + \cdots + m_5)}$$

from each component of $(\mathbf{0}, \boldsymbol{\varrho}_1, \ldots, \boldsymbol{\varrho}_5)$ to get $(\mathbf{r}_0, \ldots, \mathbf{r}_5)$. Then

$$T = \frac{1}{2}\sum_{i=0}^{5} m_i|\dot{\mathbf{r}}_i|^2, \quad V = -\sum_{i=0}^{5}\sum_{j=i+1}^{5} \frac{Gm_im_j}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad L = T - V, \tag{24}$$

where G is the gravitational constant. The code, shown in the appendix, was made particularly compact using a `C++` 3-vector class from [3].

In the DETEST model the time unit (TU) is 100 days. Distance is measured in astronomical units (AU), where 1 AU is the mean radius of the earth's orbit. The task is to integrate from given initial values up to $t = 20$ TU; at tolerance 10^{-13} we get agreement with DETEST's reference solution to around 12 decimal places.

To see how fast the solution is, the problem was integrated to $t = 200{,}000$ TU (about 55,000 earth years), with Taylor degree 20, at tolerances 10^{-13} and 10^{-14}. The two sets of results agree

to five decimal places, and some DAETS integration statistics are

Integration of Sun and 5 planets to $t = 200,000$ TU

tol	CPU secs	no. of steps	smallest step	largest step
1e-13	24.6	40855	2.66	8.32
1e-14	27.5	45619	2.39	7.65

The number of CG nodes is 1002 without CSE and 880 with CSE, or 13.9% reduction.

It is known that Pluto is locked in a, currently stable, 3:2 resonance with Neptune. This was easy to verify over short periods from our results. For the subtleties of solar system behaviour, see [6] and references therein. This article cites evidence that over very long times the system switches between regular and chaotic behaviour in an irregular way that depends critically on ICs. Hence numerical results showing linear (regular) divergence of neighbouring solutions up to some large time T—rather than exponential (chaotic) divergence — are no evidence that such behaviour will continue up to, say, time $2\,T$.

What about the given ICs? We integrated the problem at two tolerances `1e-13` and `1e-15`, recording the solutions at successive powers of 10 up to 10^8 TU (≈ 4.2 hours CPU time for each to reach 10^8) and computing the relative error in the 2-norm at these times. The results, see Figure 8, show non-chaotic behaviour up to that point.

5. Conclusions and further work

For two significant applications to do with DAEs, we have shown that differentiation of expressions, commonly done symbolically with the help of a computer algebra system, can be done efficiently and simply by AD.

First, for the Dummy Derivatives index reduction method a theoretical scheme is given that applies in principle to preparing a DAE for solution by any standard DAE or ODE initial value code. DD-switching, which moves from one mode (local coordinate system) to another, is at the housekeeping level just a change of the size- DOF set S of indices (j, l) that define the state vector.

The scheme reduces order and index together, so one need not pre-reduce to first-order form. Finally, following this paper's theme, differentiating DAE components f_i selectively (some more than others) does not need symbolic algebra; it can be done by standard AD methods of treating them as truncated power series.

We have proof-of-concept implementations in MATLAB and C++. It remains to be seen whether the scheme can be made efficient as a practical tool. For DAEs from industrial applications that may need to switch among very many modes, it may (as in the more general case of hybrid systems) be worth keeping a run time data base of modes used, if this can speed up re-entry to a mode that has been met before.

Second, we have shown that for a DAE, all or part of whose equations $f_i = 0$ derive from the Lagrangian L of a mechanical system, producing the f_i from L can be done by pure AD without symbolic algebra. The theory was illustrated by simulation examples: a constrained mechanical system, a forced pendulum as a prescribed-path control problem, and an ODE of planetary motion.

The method of directly solving from a Lagrangian by overlaying one AD type on another might be used with other DAE solvers and AD tools. However our infrastructure, of DAETS with `FADBAD++` and the Lagrangian facility has several advantages:

- For any SA-friendly DAE, the user leaves both conversion of L to equations of motion, and index/order reduction of the resulting DAE, to be done by DAETS automatically.

- It avoids large symbolic expressions that a computer algebra system typically generates when converting to a form suitable for integration by a standard ODE/DAE solver.
- Constrained 'first kind' Lagrangians in cartesian coordinates are often simpler to formulate than unconstrained 'second kind' ones in other coordinates. For a high-index DAE solver such as DAETS, possible obstacles posed by index reduction and DD-switching are absent, and constrained systems are as easy to solve as unconstrained, which makes 'first kind' forms more attractive.
- It can be programmed in a way that is intuitive and close to the mathematics, which using cartesian coordinates is itself more readable and accessible.
- It gives remarkably fast code in the cases we have tried (which can be seen from the DAETS statistics of the animations at [13]).

Current work is exploring our Lagrangian approach on a variety of research and engineering problems, and in particular rigid-body mechanics simulations and control problems. We are particularly interested in hybrid systems, because of their importance in industrial engineering.

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Notes

1. For instance `q + 1` references a sub-array of `q` starting at `q[1]`.
2. Enright and Pryce [2] cite nonexistent reference '11' which should be '10' and is the Zonneveld work.

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Appendix. Extract from code for planetary problem

This is the `fcn()` code for 3D motion of $n+1$ gravitating bodies, where body 0 is the Sun and the x,y,z positions of the other bodies are relative to it. It was specialized to the problem in Example 4.3 by providing suitable input to the main program, not shown. Note this function is not restricted to 5 bodies: their number and masses are passed as parameters.

```
template <typename T>
void fcn( T t, const T *z, T *f, void *pp ) {
  const double *param = (double *)pp;
  const int  nMASS = param[0],
                n = nMASS-1;
  const double   G = param[1];
  const double  *m = param + 2,
         *mplanet  = m+1;                // the masses EXCLUDING the Sun
  const double Mtotal = (m + nMASS)[0];  // total mass, calculated in main program

  typedef Vector3D< B<T> > vec3;
  vector< B<T> > q(3*n), qp(3*n);  // independent variables
  B<T> L;                          // for storing Lagrangian
  // { ... } ensures all intermediate variables go out of scope
  {
    init_q_qp(z,q,qp);  // setup q, qp

    // Convert to a vector of 3D vectors.
    vector< vec3 >  Q(n), Qp(n);
    for (int imass=0; imass<n; imass++) {
      Q[imass]  = vec3( q [3*imass],  q[3*imass+1], q [3*imass+2] );
      Qp[imass] = vec3( qp[3*imass], qp[3*imass+1], qp[3*imass+2] );
    }

    vector< vec3 > R(nMASS), Rp(nMASS);
    R[0] = Rp[0] = vec3(0,0,0);
    for (int imass=0; imass<n; imass++) {
```

```
28        R [0] -= mplanet[imass]*Q [imass]; Rp[0] -= mplanet[imass]*Qp[imass];
29      }
30      R [0] /= Mtotal; Rp[0] /= Mtotal;
31
32      // then set r_1, ..., r_n and their derivatives:
33      for (int imass=1; imass<nMASS; imass++) {
34        R [imass] = Q [imass-1]+R [0]; Rp[imass] = Qp[imass-1]+Rp[0];
35      }
36
37      // Compute KE and PE in terms of r and rp arrays
38      B<T> KE = 0;
39      for (int imass=0; imass<nMASS; imass++)
40        KE += m[imass] * Rp[imass]*Rp[imass];
41      KE *= 0.5;
42
43      // Potential Energy (sum of all mass-to-mass PEs, -> -oo as bodies
44      // become close)
45      B<T> PE = 0;
46      for (int imass=0; imass<nMASS; imass++)
47        for (int jmass=imass+1; jmass<nMASS; jmass++)
48          PE -= m[imass] * m[jmass] / norm(R[imass]-R[jmass]);
49      PE = G*PE; // bring in gravitational constant
50
51      L = KE-PE;
52    }
53    vector<B<T> > C; // dummy constraint variable
54    setupEquations(L,z,q,qp,C,f);
55  }
```